



Inventor: DiFoggio et al.
Title: Method and Apparatus For Chemometric...
Serial No.: 10/801,267; Filed: March 16, 2004
Docket No.: 584-37008-USCP

1/19

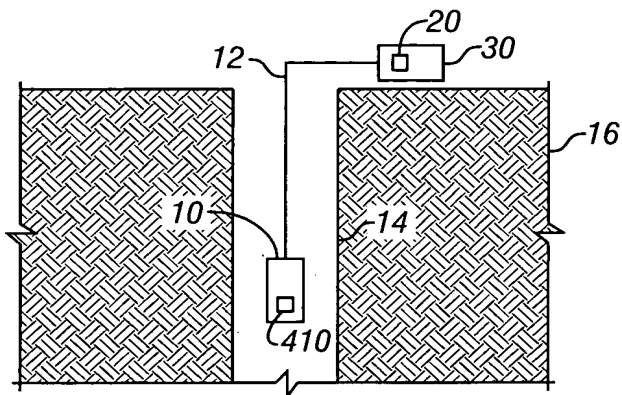


FIG. 1

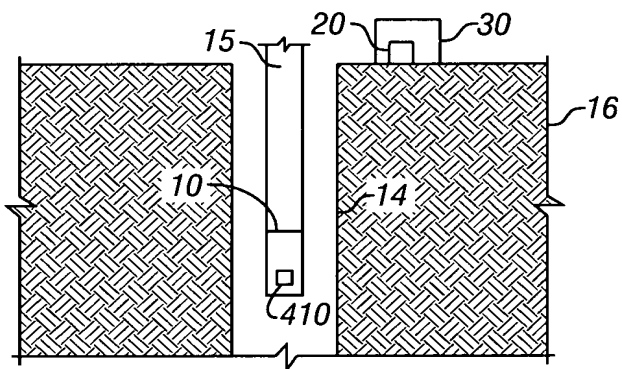


FIG. 2

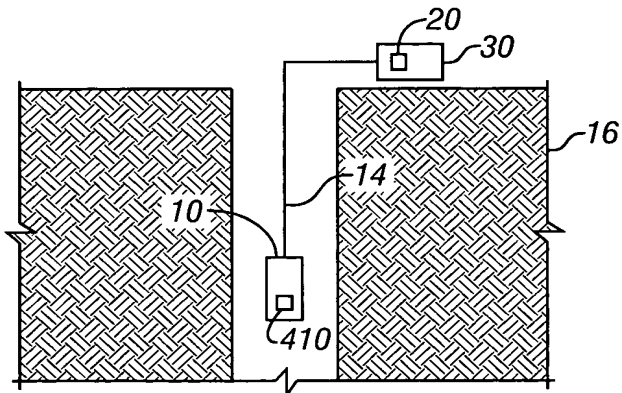
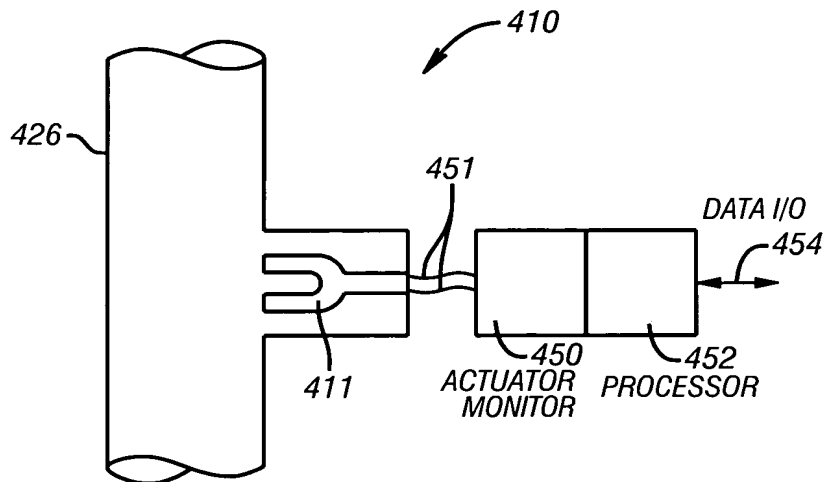
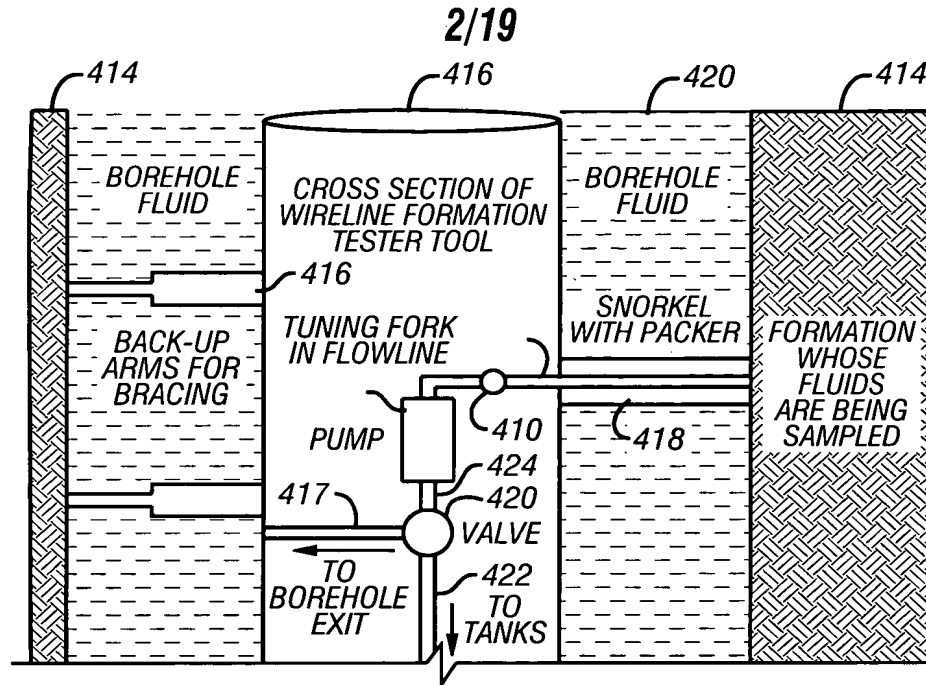


FIG. 3



3/19

*CREATE SYNTHETIC DATA SET BY EXPERIMENTAL DESIGN
USING SEVERAL VALUES OF EACH PROPERTY*

610

*CREATE CHEMOMETRIC EQUATIONS THAT CORRELATE
FLUID PROPERTIES TO IMPEDANCE VS. FREQUENCY*

620

*APPLY THESE EQUATIONS TO MEASURED RESONATOR
RESPONSE SO AS TO ESTIMATE FLUID PROPERTIES*

630

*ALTERNATIVELY, USE CHEMOMETRIC ESTIMATES AS
STARTING VALUES IN NON-LINEAR LEAST-SQUARE FIT*

640

FIG. 6

4/19

Density

Regression Summary for Dependent Variable: g/cc (Synthetic Impedance Data.sta)

$R = .99263581$ $R^2 = .98532585$ Adjusted $R^2 = .98514010$

$F(1,79) = 5304.6$ $p < 0.0000$ Std. Error of estimate: .05053

	Beta	Std. Err.	B	Std. Err.	t(79)	p-level
Intercept			-10.0370	0.151558	-66.2254	0.00E+00
1/FLZD1	0.992636	0.013629	32.4538	0.445593	72.8328	0.00E+00

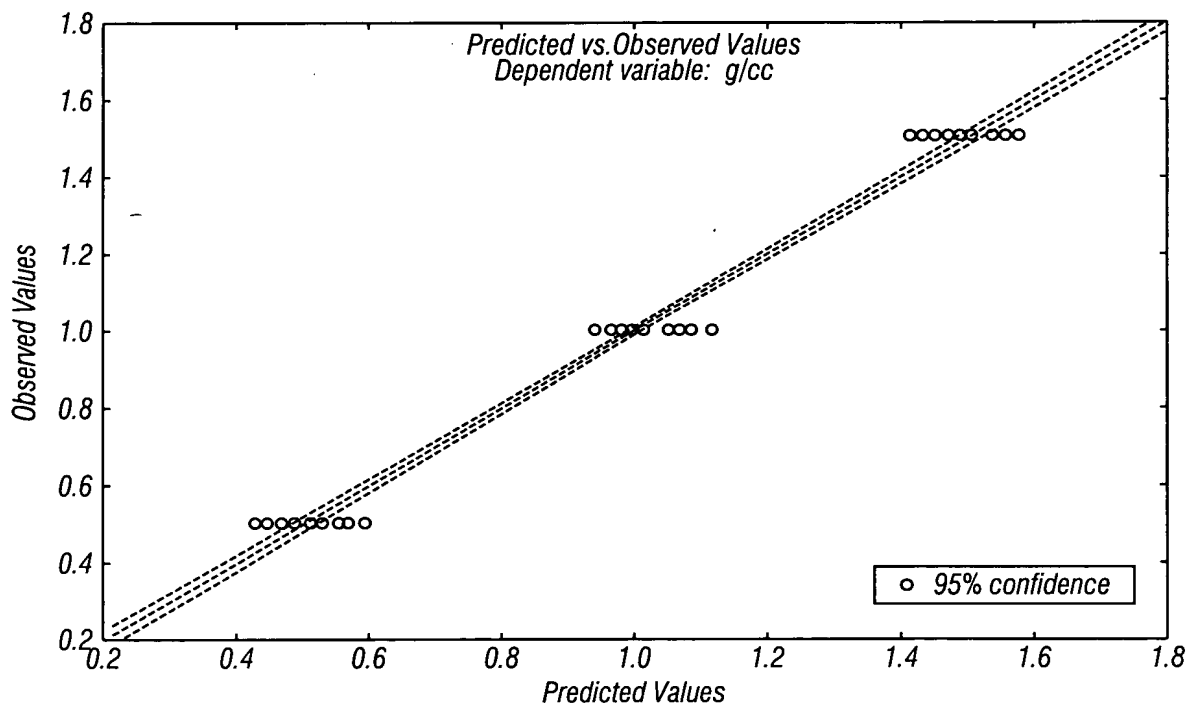


FIG. 7A

5/19

Density

Regression Summary for Dependent Variable: g/cc (Synthetic Impedance Data.sta)

R= .99909311 R²= .99818705 Adjusted R²= .99801321

F(7,73)=5741.8 p<0.0000 Std. Error of estimate: .01848

	Beta	Std. Err.	B	Std. Err.	t(73)	p-level
Intercept			-9.8709	0.08397	-117.550	0.00E+00
log(MaxD2)	0.158008	0.014018	0.0563	0.00500	11.272	1.121E-17
1/FMn_D1	0.714452	0.090942	23.2643	2.96161	7.856	2.62E-11
Cub_Min	0.728493	0.114662	100.5412	15.82487	6.353	1.61E-08
Cub_Avg	-0.738300	0.119953	-98.6059	16.02067	-6.155	3.67E-08
Min_D2	0.046837	0.012946	346.1813	95.68643	3.618	5.44E-04
1/FLZD1	0.323058	0.090546	10.5622	2.96037	3.568	6.40E-04
Sqr_Min	0.106546	0.042182	3.0742	1.21708	2.526	1.37E-02

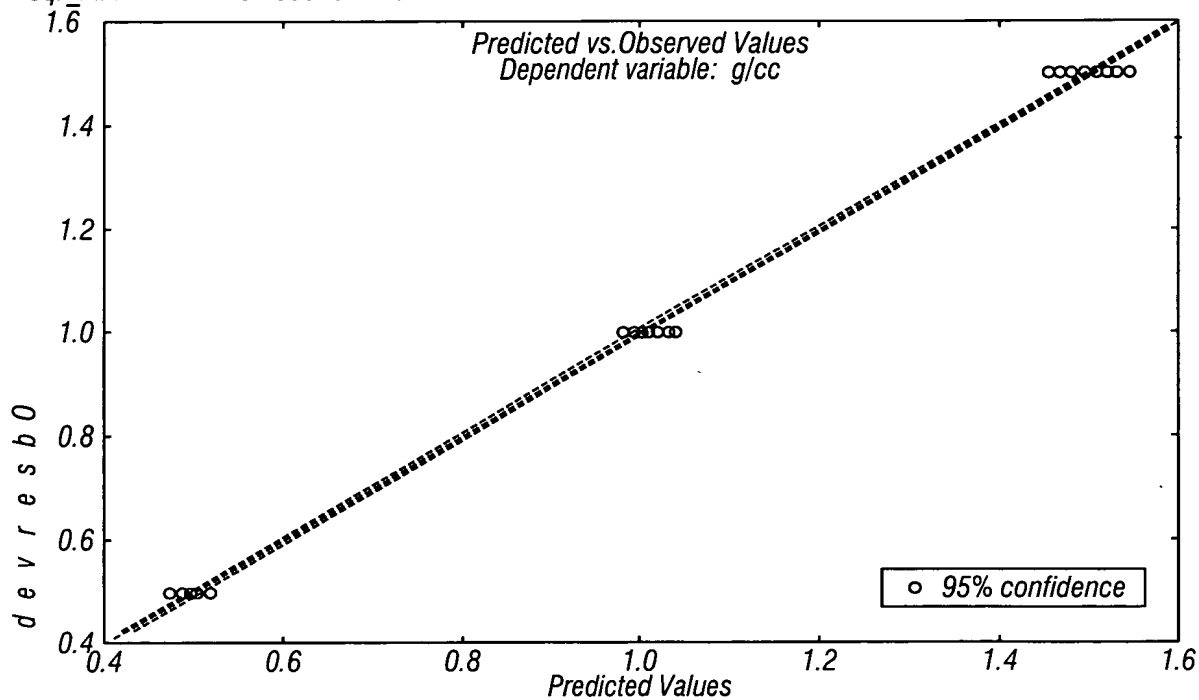


FIG. 7B

6/19

Density

Regression Summary for Dependent Variable: g/cc (Synthetic Impedance Data.sta)

$R = .99970856$ $R^2 = .99941721$ Adjusted $R^2 = .99933396$

$F(10,70) = 12004$. $p < 0.0000$ Std. Error of estimate: .01070

	Beta	Std. Err.	B	Std. Err.	t(70)	p-level
Intercept			-10.1349	0.04869	-208.130	0.000000E+00
log(MaxD2)	0.086694	0.006457	0.0309	0.00230	13.426	4.807740E-21
1/Min_D2	0.117544	0.009139	0.0000	0.00000	12.862	4.117729E-20
1/Max_D1	0.052427	0.006022	0.0000	0.00000	8.706	9.173387E-13
AvgD1	-0.047915	0.006490	-93.3906	12.64923	-7.383	2.489016E-10
1/FMn_D2	0.447306	0.082745	13.8455	2.56121	5.406	8.448959E-07
1/FMn_D1	0.446249	0.086245	14.5310	2.80834	5.174	2.086349E-06
1/Max	0.438247	0.106496	0.0261	0.00633	4.115	1.041422E-04
1/Min	-0.432207	0.108163	-0.0218	0.00547	-3.996	1.573313E-04
1/FLZD1	0.186323	0.047327	5.8908	1.49630	3.937	1.924973E-04
Log(Max)	0.071356	0.018739	0.1189	0.03122	3.808	2.976181E-04

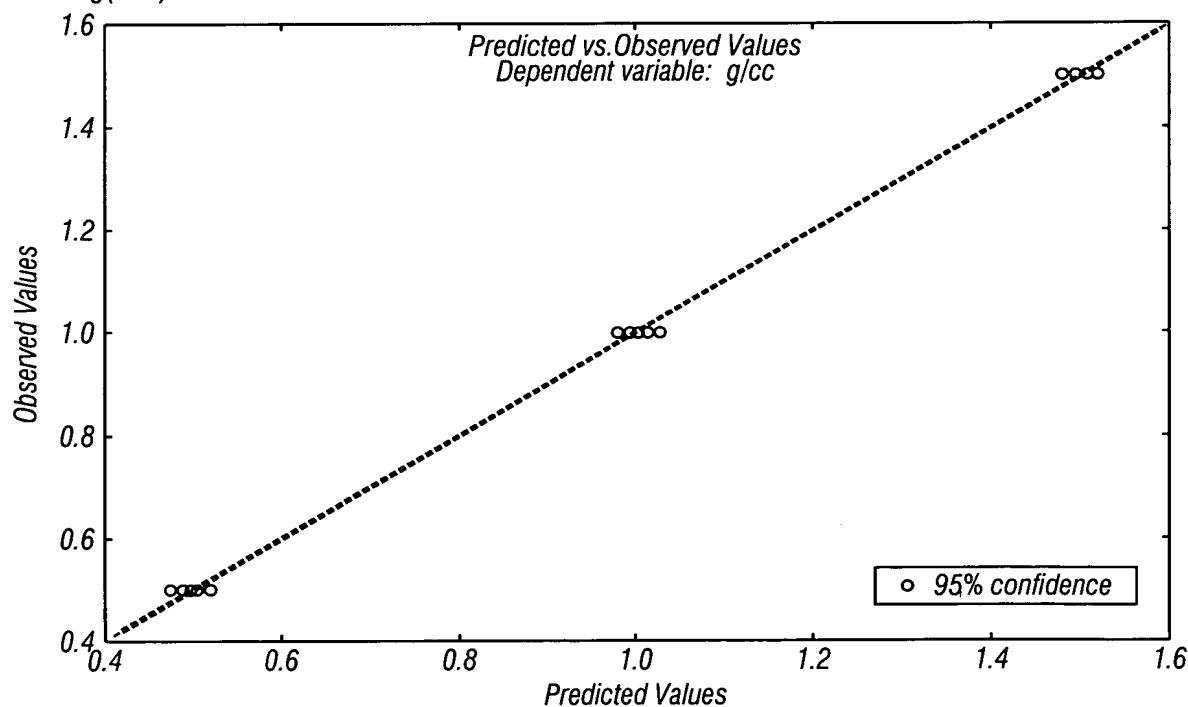


FIG. 7C

7/19

Viscosity

Regression Summary for Dependent Variable: cPs (Synthetic Impedance Data.sta)

$R = .97696409$ $R^2 = .95445882$ Adjusted $R^2 = .95206192$

$F(4,76) = 398.2$ $p < 0.0000$ Std. Error of estimate: .26970

	Beta	Std. Err.	B	Std. Err.	t(76)	p-level
Intercept			-15.694	0.9671	-16.2279	2.089853E-26
1/MinD2	-0.840896	0.035160	0.000	0.0000	-23.9160	4.151239E-37
FreqRMaxD1	0.506923	0.028371	5.662	0.3169	17.8679	6.229948E-29
MinD2	0.376456	0.033230	8268.363	729.8467	11.3289	5.432749E-18
Sqr_Min	-0.117944	0.024612	-10.112	2.1102	-4.7922	7.999455E-06

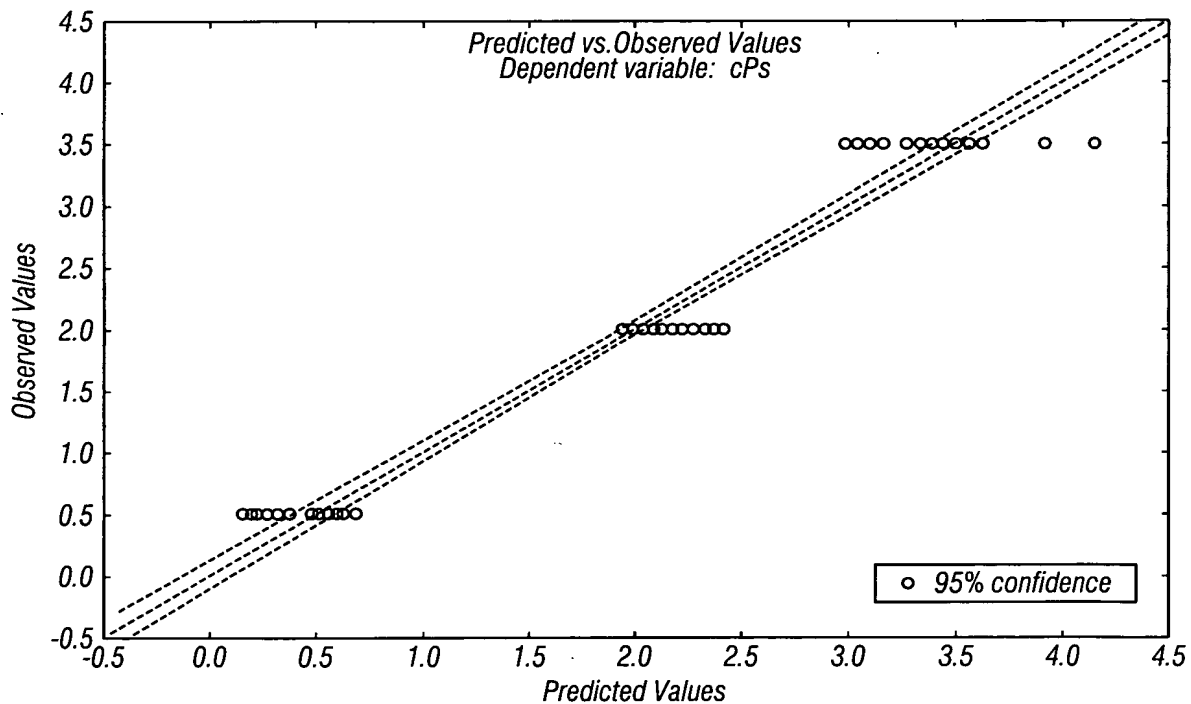


FIG. 7D

8/19

Viscosity

Regression Summary for Dependent Variable: cPs (Synthetic Impedance Data.sta)

$R = .97873578$ $R^2 = .95792372$ Adjusted $R^2 = .95511863$

$F(5,75) = 341.5$ $p < 0.0000$ Std. Error of estimate: .26096

	Beta	Std. Err.	B	Std. Err.	t(75)	p-level
Intercept			-17.653	1.214	-14.5445	1.57E-23
FreqLZeroD1	0.483355	0.029189	5.411	0.327	16.5596	9.17E-27
1/MinD2	-0.693825	0.058609	0.000	0.000	-11.8381	7.78E-19
Cub_Min	-0.169016	0.031429	-69.316	12.890	-5.3776	8.24E-07
MinD2	0.245608	0.065284	5394.464	1433.871	3.7622	3.32E-04
log(MaxD2)	-0.268470	0.097688	-0.284	0.103	-2.7482	7.50E-03

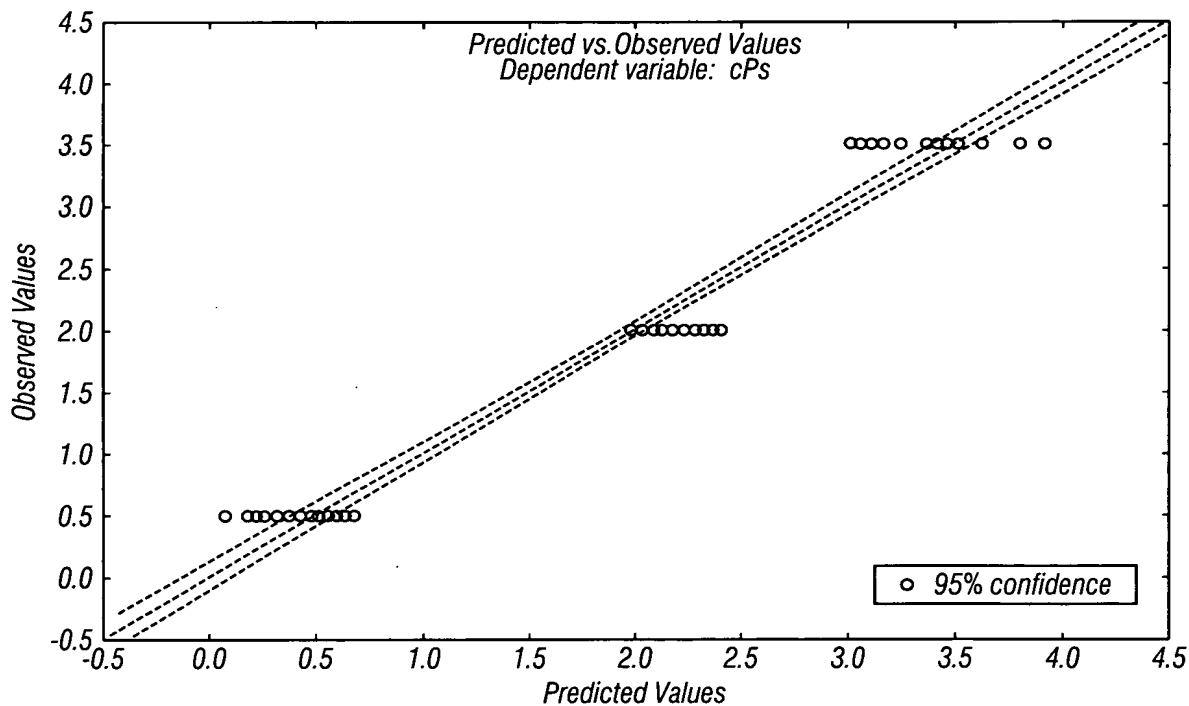


FIG. 7E

9/19

Viscosity

Regression Summary for Dependent Variable: cPs (Synthetic Impedance Data.sta)

$R = .98468409$ $R^2 = .96960276$ Adjusted $R^2 = .96757627$

$F(5,75) = 478.47$ $p < 0.0000$ Std. Error of estimate: .22181

	Beta	Std. Err.	B	Std. Err.	t(75)	p-level
Intercept			-12.938	0.8918	-14.5075	1.813627E-23
1/MinD2	-0.691176	0.043747	0.000	0.0000	-15.7994	1.434065E-25
PK	0.368418	0.029871	250.435	20.3047	12.3338	1.005152E-19
log(MaxD2)	-0.368199	0.043609	-0.390	0.0462	-8.4431	1.709891E-12
Cub_Min	-0.131400	0.023774	-53.889	9.7499	-5.5272	4.512895E-07
P27_D2	0.128036	0.028700	3078.767	690.1188	4.4612	2.817552E-05

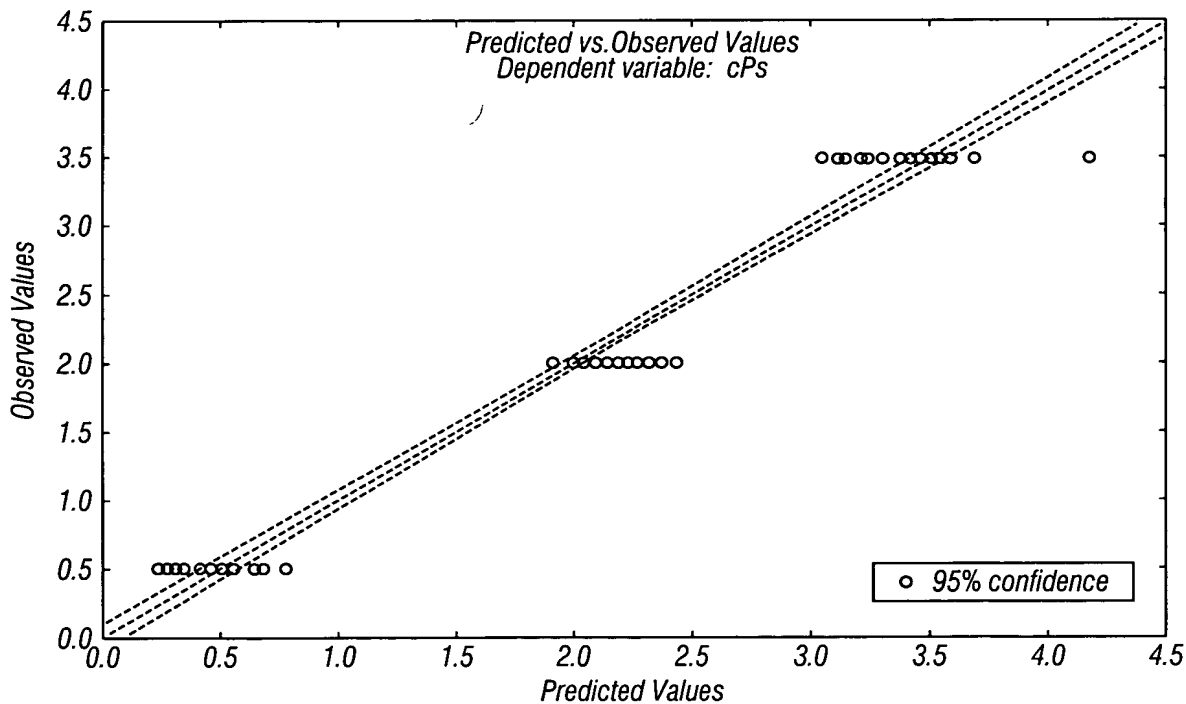


FIG. 7F

10/19

Dielectric Constant

Regression Summary for Dependent Variable: Dielectric (Synthetic Impedance Data.sta)

$R = .99511668$ $R^2 = .99025720$ Adjusted $R^2 = .98974442$

$F(4,76) = 1931.2$ $p < 0.0000$ Std. Error of estimate: 1.1857

	Beta	Std. Err.	B	Std. Err.	t(76)	p-level
Intercept			-9.15	0.581	-15.7513	1.206053E-25
AvgD1	1.37132	0.054288	75492.69	2988.616	25.2601	1.029444E-38
Sqr_Max	-1.46607	0.108461	-1157.11	85.604	-13.5170	6.567799E-22
Cub_Avg	4.64294	0.680918	17514.38	2568.600	6.8187	1.924593E-09
Cub_Max	2.46760	0.623626	-8978.25	2269.034	-3.9589	1.693159E-04

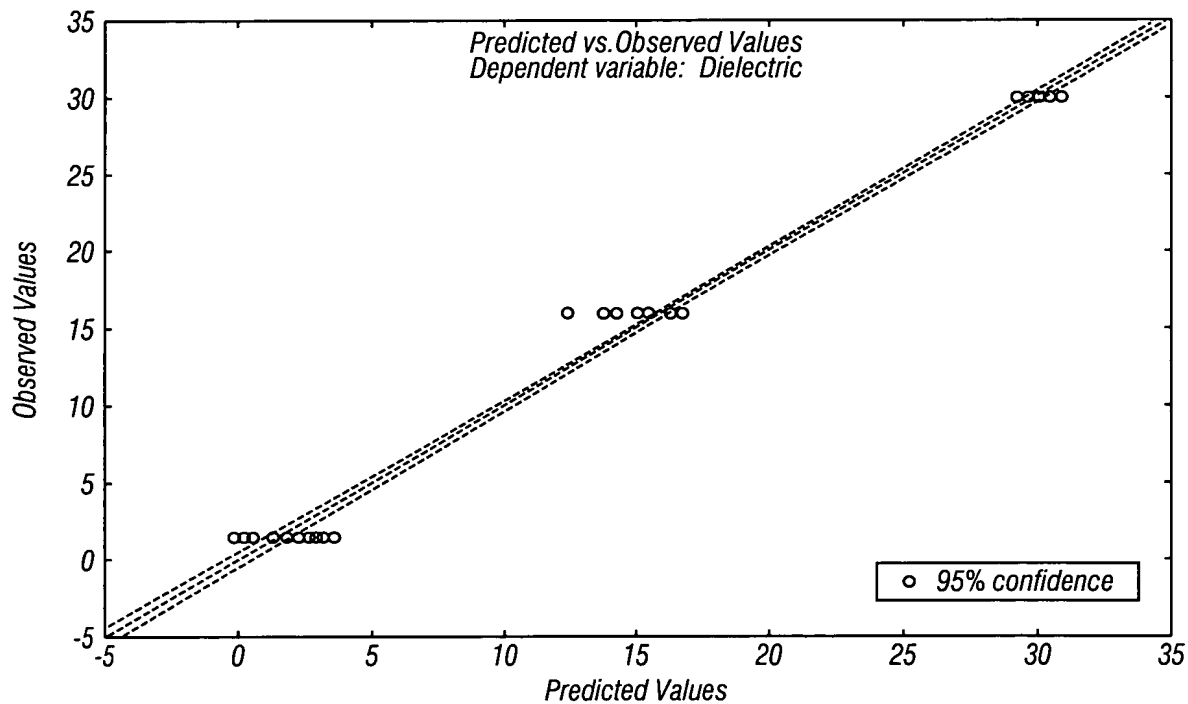


FIG. 8A

11/19

Dielectric Constant

Regression Summary for Dependent Variable: Dielectric (Synthetic Impedance Data.sta)

R = .99943711 R = .99887453 Adjusted R² = .99878328

F(6,74)=10946. p<0.0000 Std. Error of estimate: .40840

	Beta	Std. Err.	B	Std. Err.	t(74)	p-level
Intercept			-7.53	1.2377	-6.0807	4.808670E-08
AvgD1	0.66643	0.016800	36687.94	924.8812	39.6677	0.000000E+00
1/AvgD1	-0.197847	0.007860	-0.000163	0.000006	-25.1721	0.000000
Cub_Avg	2.44530	0.154098	9224.32	581.2968	15.8685	1.592333E-25
Sqr_Min	-3.33853	0.285158	-2720.66	232.3839	-11.7076	1.638646E-18
Min	1.54184	0.134232	304.33	26.4945	11.4864	4.100279E-18
Log(FMx_D1)	-0.01485	0.003953	-9.21	2.4350	-3.7556	3.421367E-04

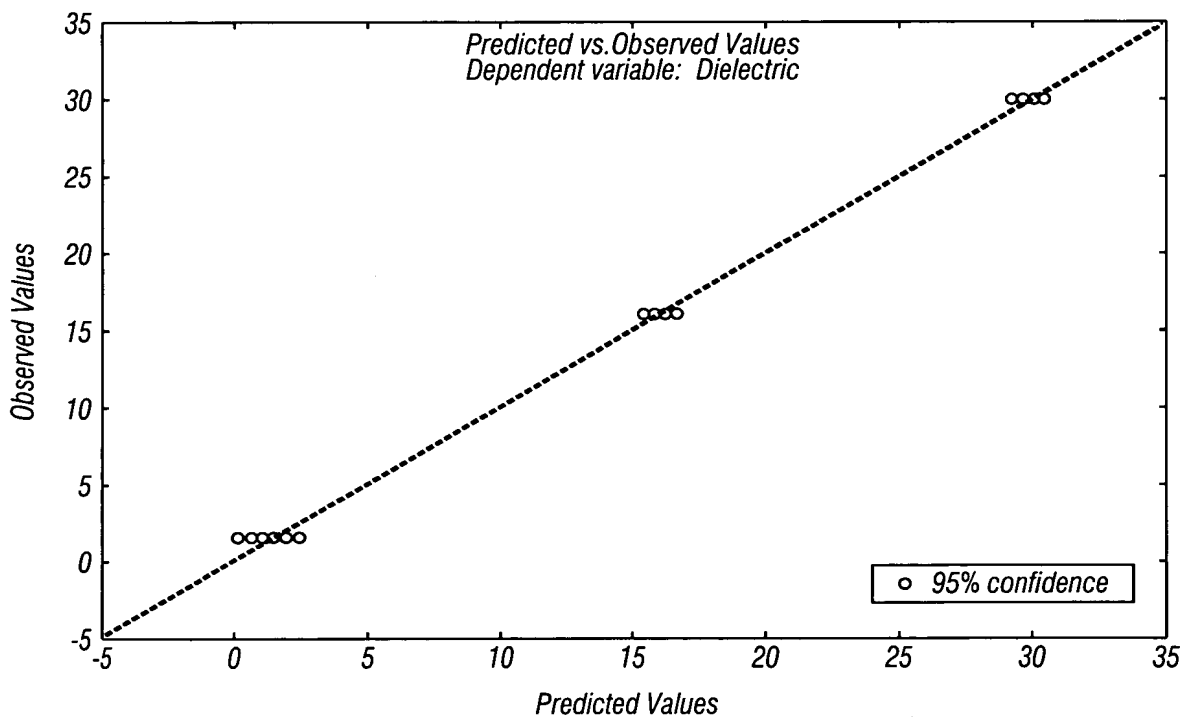


FIG. 8B

12/19

Dielectric Constant

Regression Summary for Dependent Variable: Dielectric (Synthetic Impedance Data.sta)

$R = .99901744$ $R^2 = .99803585$ Adjusted $R^2 = .99795932$

$F(3,77) = 13042$. $p < 0.0000$ Std. Error of estimate: .52890

	Beta	Std. Err.	B	Std. Err.	t(77)	p-level
Intercept			35.64	1.2392	28.7567	6.24E-43
Cub_Min	0.676927	0.005494	2638.71	21.4159	123.2124	0.00E+00
AvgD1	0.656755	0.010915	36155.19	600.9014	60.1683	0.00E+00
Log(AvgD1)	0.401660	0.011145	10.63	0.2950	36.0399	0.00E+00

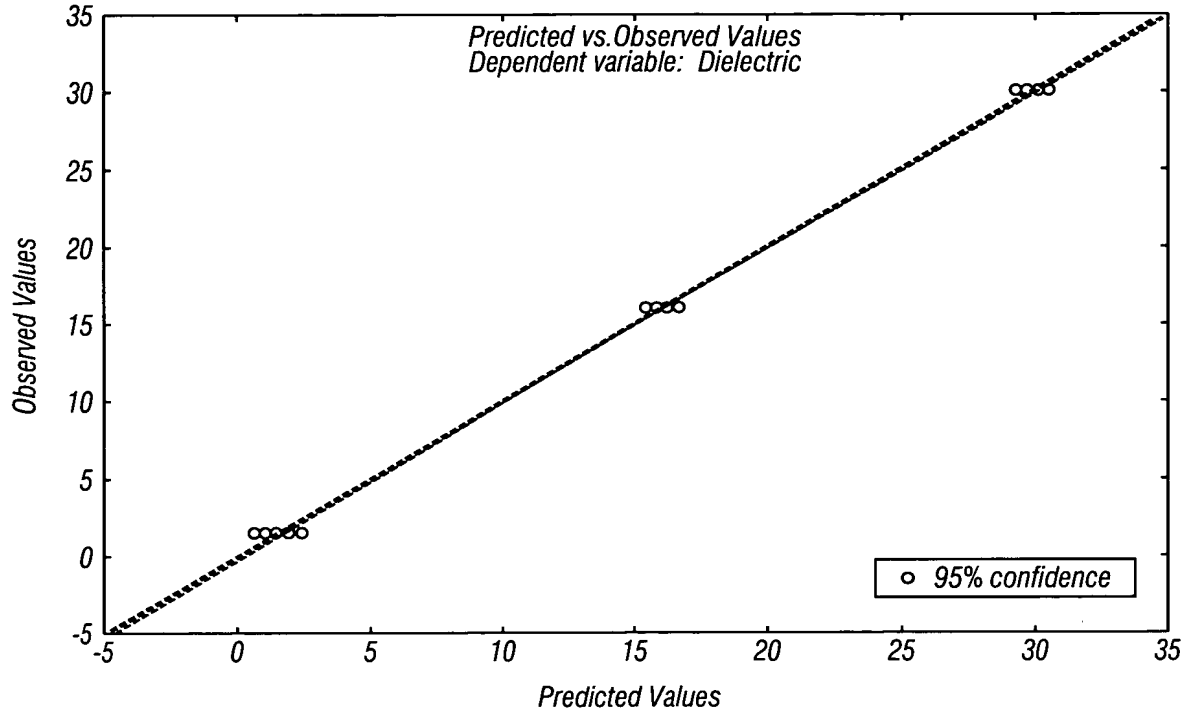


FIG. 8C

13/19

Conductivity

Regression Summary for Dependent Variable: 1/ohm*m (Synthetic Impedance Data.sta)

$R = .99825839$ $R^2 = .99651982$ Adjusted $R^2 = .99633665$

$F(3,77) = 13042$. $p < 0.0000$ Std. Error of estimate: .52890

	Beta	Std. Err.	B	Std. Err.	t(76)	p-level
Intercept			0.000112	0.000025	4.3989	3.495104E-05
Max	-3.84661	0.091676	-0.002934	0.000070	-41.9589	0.000000E+00
Min	3.86666	0.064796	0.002932	0.000123	23.9154	4.158121E-37
Cub_Min	0.47895	0.011145	0.007172	0.000970	7.3916	1.594179E-10
Log(Min)	0.37400	0.089062	0.000063	0.000015	4.1993	7.204409E-05

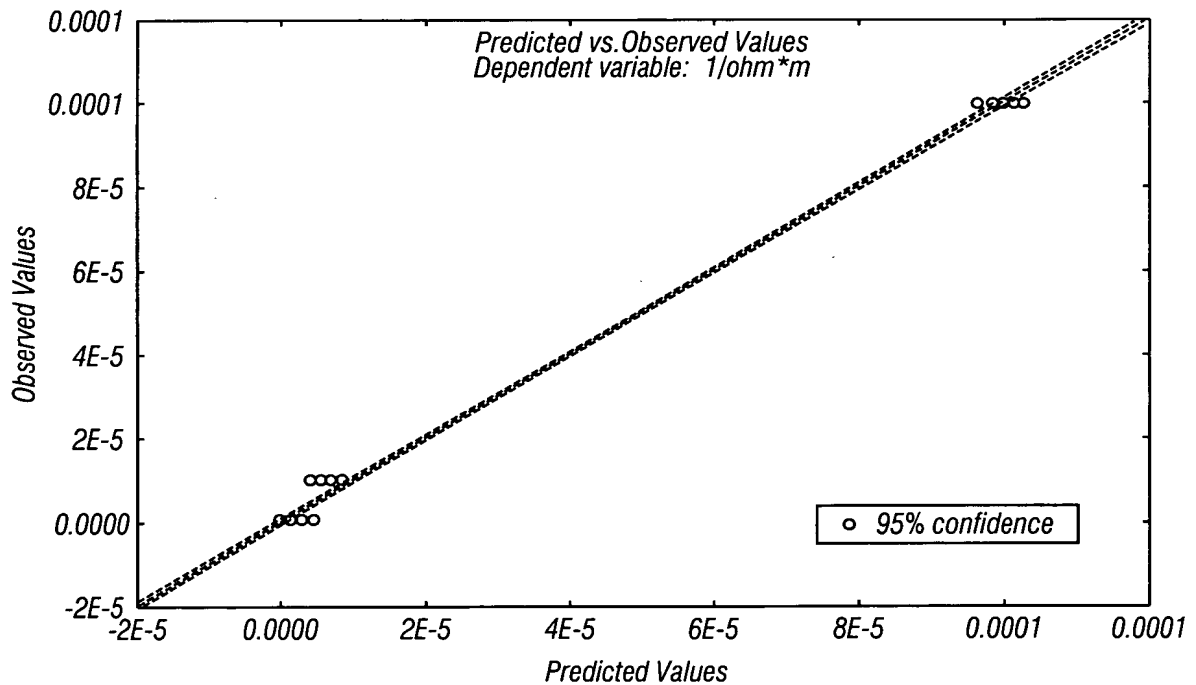
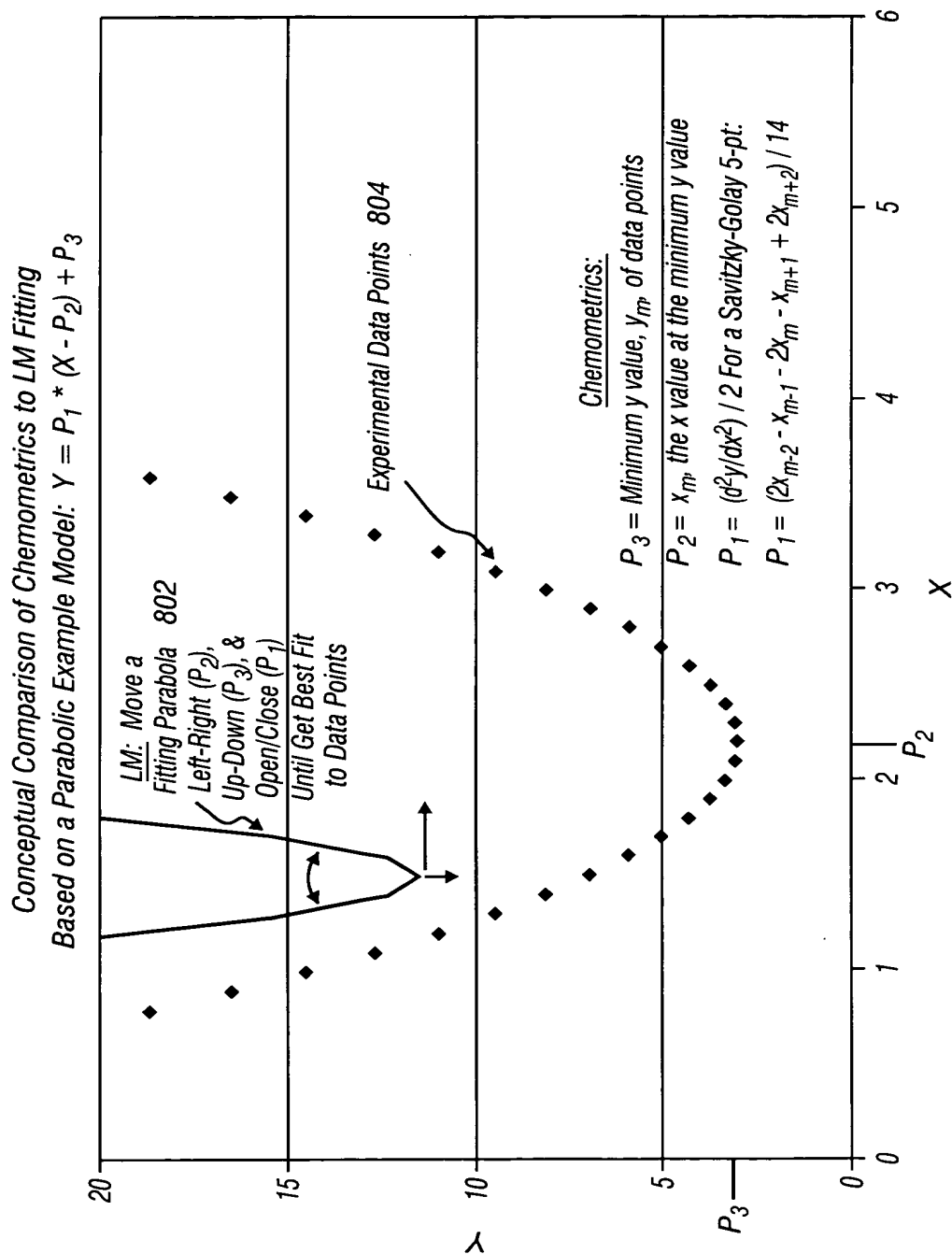


FIG. 8D

14/19

<i>Some Definitions of Variables</i>	
<i>Min</i>	<i>Minimum Impedance in Spectrum</i>
<i>Max</i>	<i>Maximum Impedance in Spectrum</i>
<i>Avg</i>	<i>Average Impedance in Spectrum</i>
<i>PK</i>	<i>Frequency of 1st Derivative Minimum Value (an inverted Peak)</i>
<i>Sqr_</i>	<i>Square of _</i>
<i>Cub_</i>	<i>Cube of _</i>
<i>Log()</i>	<i>Log 10 of</i>
<i>1/</i>	<i>Reciprocal of</i>
<i>D1</i>	<i>First Derivative of Impedance vs Frequency</i>
<i>D2</i>	<i>Second Derivative of Impedance vs Frequency</i>
<i>D3</i>	<i>Third Derivative of Impedance vs Frequency</i>
<i>MinD1=</i>	<i>Minimum of First Derivative of Impedance in Spectrum</i>
<i>MaxD1=</i>	<i>Maximum of First Derivative of Impedance in Spectrum</i>
<i>MinD2=</i>	<i>Minimum of Second Derivative of Impedance in Spectrum</i>
<i>MaxD2=</i>	<i>Maximum of Second Derivative of Impedance in Spectrum</i>
<i>1/FMn_D1</i>	<i>Reciprocal of Frequency of Minimum D1 (Inverted Peak)</i>
<i>1/FMx_D1</i>	<i>Reciprocal of Frequency of Minimum D1</i>
<i>FreqAtMinD1</i>	<i>Frequency of Minimum D1 (Inverted Peak)</i>
<i>FreqAtMaxD1</i>	<i>Frequency of Minimum D1 (May pick up small bump on either side of Inverted Peak)</i>
<i>FreqAtMinD2</i>	<i>Frequency of Minimum D2</i>
<i>FreqAtMaxD2</i>	<i>Frequency of Maximum D2</i>
<i>FreqAtMinD3</i>	<i>Frequency of Minimum D3</i>
<i>FreqAtMaxD3</i>	<i>Frequency of Maximum D3</i>
<i>FreqLMaxD1=</i>	<i>Frequency of LEFT Maximum D1 (Left of Inverted Peak)</i>
<i>FreqRMaxD1=</i>	<i>Frequency of RIGHT Maximum D1 (Left of Inverted Peak)</i>
<i>FreqLZeroD1=FLZD1 =</i>	<i>Frequency of LEFT Zero D1 (Left X-axis Crossing Point)</i>
<i>FreqRZeroD1=FLZD1 =</i>	<i>Frequency of RIGHT Zero D1 (Right X-axis Crossing Point)</i>

FIG. 8E



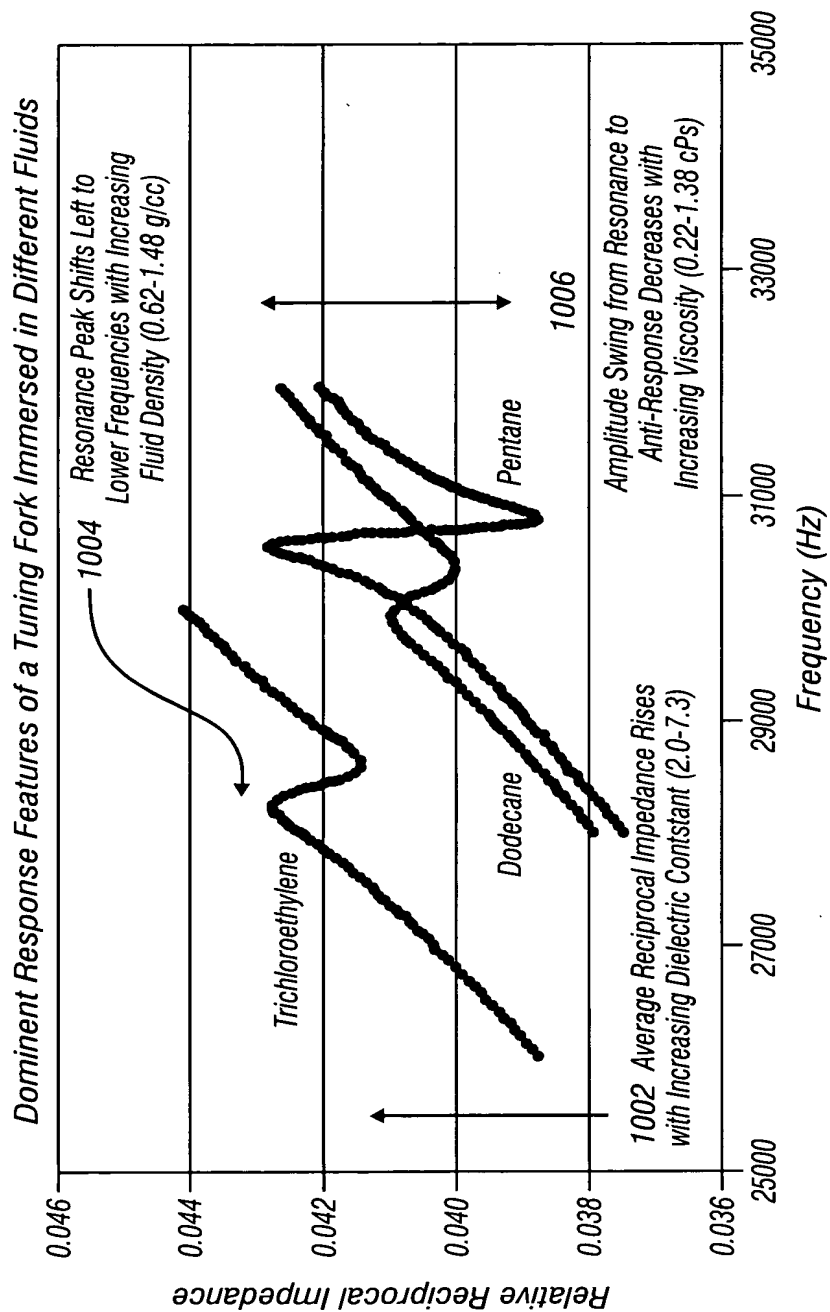


FIG. 10

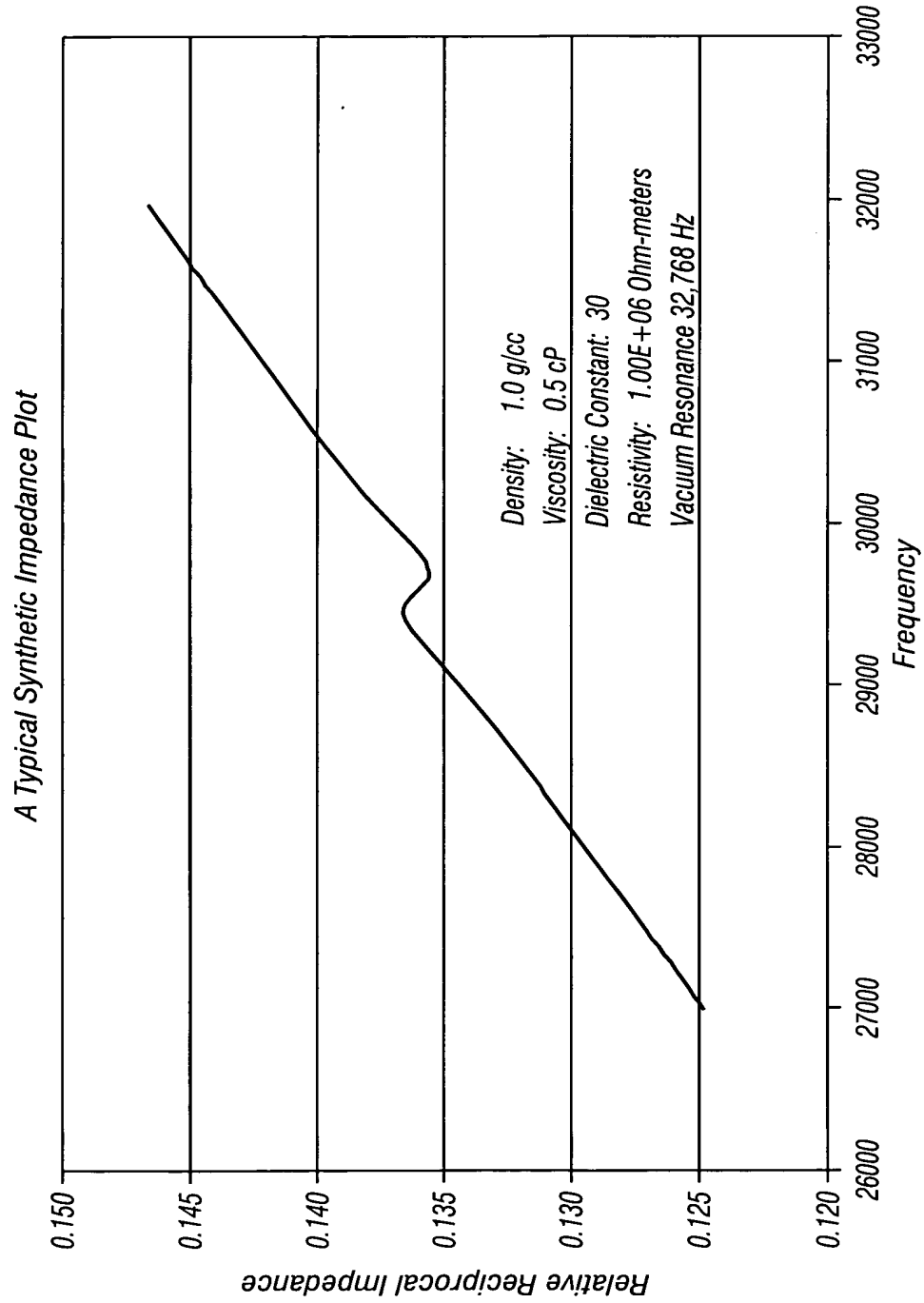


FIG. 11

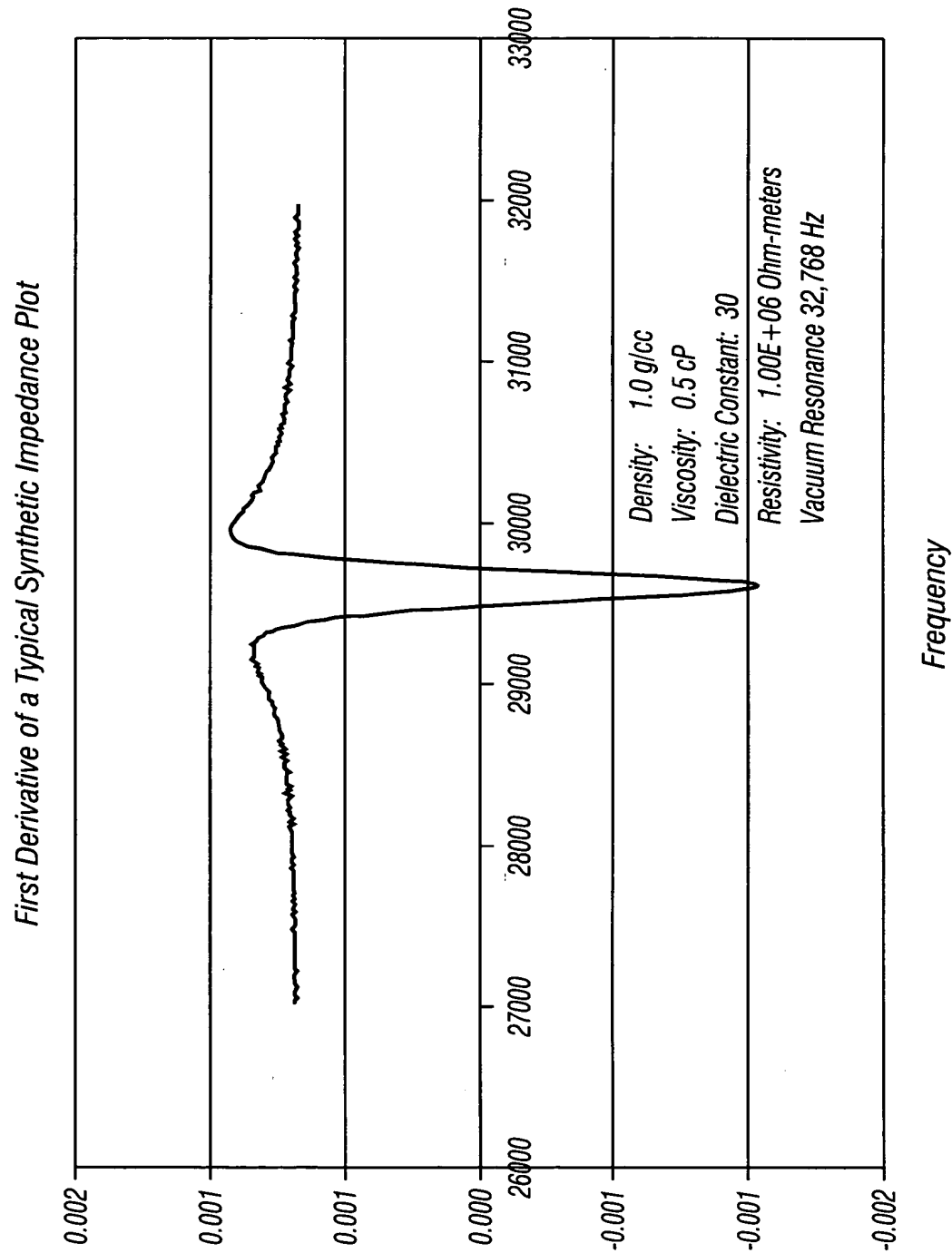


FIG. 12



FIG. 13